Design and Development of New Zinc Porphyrin Molecules as High Performing Photoacoustic Contrast Agents

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Doctor of Philosophy

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I hereby declare that the work in this thesis is based on my original work except for quotations and citations which have been duly acknowledged. I also declare that it has not been previously or concurrently submitted for any other degree at Universiti Malaysia Pahang or any other institutions.

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DEDICATION

"This thesis is dedicated to all my Teachers and Supervisors, especially Dr. Munawar Ali Munawar & Prof. Dr. Jose Rajan for providing me a source of inspiration and their countless effort, to my Father Muhammad Yasin Bhatti for his love and giving me encourage in every step of life and to my Husband Muhammad Wasif Nabeel for his patience and moral support"

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ABSTRAK

Penyelidikan doktoral ini bertujuan untuk merekabentuk dan membangunkan molekul porfirin baru sebagai agen kontras dalam pengimejan fotoakustik (PA) seperti tomografi PA dan mikroskopi PA. Untuk kejayaan pelaksanaan teknik pengimejan PA, agen kontras yang mempamerkan koefisien PA yang besar adalah salah satu keperluan penting. Banyak bahan, sama ada biomolekul endogen seperti hemoglobin, deoxyhaemoglobin, melanin atau bahan-bahan eksogen seperti molekul organik, kluster atau nanokristal didapati menunjukkan kesan PA. Walau bagaimanapun, ia sama ada dihad oleh koefisien PA yang lemah, kedalaman penembusan yang lemah atau ketoksikan. Pengembangan molekul PA baru adalah terhad kerana faktor-faktor yang mempengaruhi kesan PA jarang diteliti secara sistematik, mengakibatkan kekurangan panduan untuk reka bentuk molekul agen kontras PA. Dalam tesis ini, hipotesis bahawa kesan PA yang besar boleh dicapai jika getaran kumpulan molekul atau berfungsi terletak di atas atom yang membentuk orbital molekul tidak dihuni paling rendah dapat dimanipulasi sedemikian rupa sehingga kekuatan pengayun dari getaran tersebut meningkat pada pengubahsuaian kimia yang sesuai, maka sebahagian besar foton yang teruja dapat disejukkan melalui pelepasan fonon. Dengan menggunakan Zn(II)porfirin sebagai sistem model, sebilangan besar molekul dimodelkan menggunakan teori berfungsi ketumpatan (DFT) semasa berdasarkan andaian di atas dan sifat asas dan keadaan teruja dikaji secara sistematik dengan menggunakan kaedah hibrid tiga parameter Becke dengan gradien korelasi berfungsi (B3LYP) Lee, Yang, dan Parr dan teras-teras berpotensi diperbetulkan yang berkesan menggunakan LANL2DZ dan 6-31G(d) dalam pakej program Gaussian 09W. Telah diperhatikan bahawa kumpulan-kumpulan berfungsi dalam kumpulan fenil kurang resonans yang melekat pada teras porfirin menguatkan kekuatan ayunan kelompok alkoksi – variasi sistematik dalam koefisien penyerapan mod C-H vibrational juga diperhatikan dengan perubahan relatif dalam resonans kumpulan molekul berlabuh. Dipengaruhi pemerhatian tersebut, empat molekul molekul Zn(II)porfirin (RJ-C_n-MY_m, di mana n= 12 atau 8 dan m= 1-4) telah disintesis dengan hasil yang baik melalui pengoksidaan berasaskan asid, pemeluwapan Knoevenagel, pemeluwapan MacDonald (2+2), brominasi, logam, nyahlindung dan reaksi gandingan Sonogashira. Struktur molekul dikaji menggunakan spektroskopi NMR, MS, dan FTIR manakala ciri-ciri optik dikaji dengan kaedah spektroskopi penyerapan UV-Vis, spektroskopi fotopendarkilau dan pengiraan foton tunggal yang berkorelasi; sementara sifat-sifat PA dikaji dengan kaedah spektroskopi fotoakustik. Koefisien penyerapan menurun mengikut susunan RJ-C_{12}-MY_1> RJ-C_{12}-MY_2> RJ-C_{12}-MY_3> RJ-C_8-MY_4; oleh itu variasi yang serupa dalam isyarat PA telah diramalkan. Ramalan teori telah disahkan oleh ukuran koefisien PA dengan tomografi PA. Koefisien PA dan keamatan tomografi menurun mengikut susunan RJ-C_{12}-MY_1> RJ-C_{12}-MY_2> RJ-C_{12}-MY_3> RJ-C_8-MY_4, seperti yang diramalkan oleh DFT. Pengelasan molekul terperinci dalam menentukan ciri-ciri optoelektronik seperti kepupusan koefisien molar keadaan asas, kepupusan koefisien molar keadaan teruja, hasil kuantum pendarfluor dan masa hayat keadaan teruja molekul Zn(II)porfirin yang baru disintesis diperiksa bagi menunjukkan korelasi positif antara tahap tenaga getaran, koefisien kepupusan molar, keadaan pemancaran fonon dan kesan PA. Koefisien PA yang besar diperhatikan bagi RJ-C_{12}-MY_1 memberikan peningkatan PA sebanyak ~7 kali ganda berbanding dengan ZnTPP yang digunakan sebagai rujukan adalah lebih tinggi daripada molekul kecil sedia ada. Di samping menawarkan molekul unggul untuk tomografi PA tesis dan kriteria yang diterima pakai akan membolehkan rekabentuk molekul yang lebih mudah dengan ciri-ciri fotoakustik superior dan lain-lain ciri optik tidak linear.

ABSTRACT

This doctoral research aims to design and develop new porphyrin molecules as contrast agents in photoacoustic (PA) imaging (PAI) such as PA tomography and PA microscopy. For successful implementation of PAI techniques, contrast agents exhibiting large PA coefficients are one of the essential requirements. Many materials, either endogenous biomolecules such as haemoglobin, deoxyhaemoglobin, melanin or exogenous materials such as organic molecules, clusters or nanocrystals are shown to exhibit PA effects. However, they are either limited by poor PA coefficients, poor penetration depths or toxicity. Development of new PA molecules is limited because the factors influencing the PA effect have rarely been systematically studied, resulting in a lack of guidance for the design of molecular PA contrast agents. In this thesis, it is hypothesized that large PA effects could be achieved if vibrations of the molecular or functional groups lying above the atoms composing the lowest unoccupied molecular orbitals could be manipulated in such a way that the oscillator strength of those vibrations increase upon suitable chemical modification, then a large portion of the excited photons can be thermalized via phonon emission. By using Zn(II)porphyrin as a model system, a large number of molecules were modelled using state of the art density functional theory (DFT) based on the above assumption and their ground and excited state properties were studied systematically by using the Becke's three-parameter hybrid method with the Lee, Yang, and Parr gradient corrected correlation functional (B3LYP) with the effective core potential employing basis sets of LANL2DZ and 6-31G(d) using the Gaussian 09W program package. It was observed that less resonating functional groups in a phenyl group attached to the porphyrin core amplify the oscillation strengths of the alkoxy groups – a systematic variation in the absorption coefficients of the C-H vibrational modes was observed with relative change in the resonance of the molecular groups anchored. Motivated from this result, representative four Zn(II)porphyrin molecules (RJ-C_n-MY_m, where n = 12 or 8 and m = 1 – 4) were synthesized in good yields by acid-catalyzed oxidation, Knoevenagel condensation, MacDonald (2+2) condensation, bromination, metalation, deprotection, and Sonogashira coupling reactions. Structure of the molecules were studied by NMR, Mass Spectrometry, and FTIR spectroscopy; optical properties were studied by UV-Vis absorption spectroscopy, photoluminescence spectroscopy, and time-correlated single photon counting; and PA properties were studied by photoacoustic spectroscopy. The absorption coefficient decreased in the order of RJ-C_{12}-MY_1> RJ-C_{12}-MY_2> RJ-C_{12}-MY_3 > RJ-C_8-MY_4; and therefore, a similar variation in the PA signals was predicted. Theoretical predictions were validated by PA coefficients measurements and PA tomography. The PA coefficients and tomographic intensities decreased in the order RJ-C_{12}-MY_1> RJ-C_{12}-MY_2> RJ-C_{12}-MY_3 > RJ-C_8-MY_4, as predicted by DFT. The detailed molecular characterizations in determining the nature of optoelectronic properties i.e.; ground state molar extinction coefficients, excited state molar extinction coefficients, fluorescence quantum yields and excited state lifetimes of newly synthesized Zn(II)porphyrin molecules were examined in order to show the positive correlation between vibrational energy levels, molar extinction coefficients, phonon emitting states and PA effect. Large PA coefficients were observed for the RJ-C_{12}-MY_1, providing an up to ~7-fold PA enhancement over that of ZnTPP used as a reference, which is superior to that of the existing small molecules. Besides offering a superior molecule for PA tomography, the present thesis and criterion adopted here would enable to design simpler molecules with superior photoacoustic and other nonlinear optical properties.

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LIST OF SYMBOLS

α	Alpha
β	Beta
cm	Centimetre
Δ	Chemical shift
C_e	Concentration of excited state molecules
P	Density
R	Electron position
eV	Electron volt
λ_{em}	Emission wavelength
E_g	Energy-gap
λ_{ex}	Excitation wavelength
Fs	Femtosecond
ε_e	First excited state molar extinction coefficient
Φ_f	Fluorescence quantum yields
C_g	Ground state concentration
ε_g	Ground state molar extinction coefficient
Γ	Grüneisen coefficient
$t_{1/2}$	Half-life
Hz	Hertz
I	Incident photon fluence
∇^2	Laplacian operator
MHz	Megahertz
µJ	Microjoules

µm	Micrometre
mJ	Millijoules
mL	Millilitre
Mm	Millimeter
mmol	Millimole
Ms	Millisecond
M	Molar
E	Molar extinction coefficient
Nm	Nanometre
Ns	Nanosecond
k_{nr}	Non-radiative decay
F	Oscillation strengths
Ppm	Parts per million
Φ_{ph}	Phosphorescence quantum yield
π	Pi
Pm	Picometer
Ps	Picosecond
H	Plank constant
Φ_{nr}	Quantum yield for non-radiative decay
k_r	Radiative decay
N	Refractive index
$^1\tau$	Singlet excited state life time
C_p	Specific heat of the medium at constant pressure
C_V	Specific heat of the medium at constant volume

C	Speed of light
$\Delta\nu_1$	Splitting between excited states Q(1,0) and Q(0,0) vibrational bands
$\Delta\nu_2$	Splitting between ground states Q(0,0) and Q(1,0) vibrational bands
$\Delta\nu$	Stokes shift
α	Thermal expansion coefficient/ Linear absorption coefficient
V_s	Velocity of sound
W	Watt
Ψ	Wave function
λ	Wavelength

LIST OF ABBREVIATIONS

B3LYP	Becke, 3-parameter, Lee-Yang-Parr
($Pd(PPh_3)_2Cl_2$)	Bis(triphenylphosphine)palladium(II)chloride
BODIPY	Boron-Dipyrromethene
^{13}CNMR	Carbon Nuclear Magnetic Resonance
$CHCl_3$	Chloroform
CI	Configuration Interaction
CuI	Copper iodide
CAMB3LYP	Coulomb attenuated-B3LYP
CC	Coupled-Cluster
CCSD	Coupled Cluster with single and double excitations
DFT	Density Functional Theory
$CDCl_3$	Deuterochloroform
CD_3OH	Deuteromethanol
DDQ	2,3-dichloro-5,6-dicyano-1,4-benzoquinone
CH_2Cl_2 or DCM	Dichloromethane
DMF	Dimethylformamide
DZ	Double Zeta
E_{em}	Emission energy
EtOAc	Ethyl acetate
E_{ex}	Excitation energy
S_1	Excited singlet state
FDA	Food and Drug Administration
FTIR	Fourier Transform Infrared
GTOs	Gaussian type orbitals
GUI	Graphical user interface

S_0	Ground state
HF	Hartree-Fock
HOMO	Highest Occupied Molecular Orbital
HRMS	High Resonance Mass Spectroscopy
HK	Hohenberg-Kohn
HI	Hydriodic acid
HCl	Hydrochloric acid
HBr	Hydrogen bromide
H_2O_2	Hydrogen peroxide
ICG	Indocyanine green
IR	Infrared
IEF-PCM	Integral Equation Formalism Polarizable Continuum Model
IC	Interconversion
IUPAC	International union for pure and applied chemistry
ISC	Intersystem crossing
LR-TD-DFT	Linear response Time-dependent Density Functional Theory
LANL2DZ	Los Alamos National Laboratory (LANL) ECP with Double Zeta valence
LUMO	Lowest Unoccupied Molecular Orbital
$MgSO_4$	Magnesium sulfate
MATLAB	MATrix LABoratory
H_2TMP	meso-tetramethylporphyrin
H_2TPP	meso-tetraphenylporphyrin
$M^{II}(L)(CO)$	Metal ligand cobalt
MX_2	Metal salts
MLCT	Metal to ligand charge transfer
CH_3OH or MeOH	Methanol

MP2	Møller-Plesset Perturbation
NBS	*N*-bromosuccinimide
nBuLi	*n*-Butyllithium
NCS	*N*-chlorosuccinimide
NIR	Near-Infrared
Nd:YAG	Neodymium Yttrium Aluminum Garnet
NIS	*N*-iodosuccinimide
HNO_3	Nitric acid
N_2	Nitrogen gas
N_2O_4	Nitrogen tetroxide
NO_2BF_4	Nitrosonium borofluorate
NMR	Nuclear Magnetic Resonance
OPAZ	Optical and Photoacoustic Z-Scan
OD	Optical density
$PhSeBr_3$	Phenylselenium tribromide
$PhSeCl_3$	Phenylselenium trichloride
$POCl_3$	Phosphoryl chloride
PA	Photoacoustic
PAI	Photoacoustic Imaging
PAM	Photoacoustic Microscopy
PAT	Photoacoustic Tomography
PCM	Polarizable Continuum Model
K_2CO_3	Potassium carbonate
^{1}HNMR	Proton Nuclear Magnetic Resonance
QZ	Quadruple Zeta
QC	Quantum chemical

RSA	Reverse saturable absorption
SCRF	Self-consistent reaction-field
SAT	Sitting at top
STOs	Slater type orbital
NaN_3	Sodium azide
$NaBH_4$	Sodium borohydride
NaOH	Sodium hydroxide
TBAF	Tetrabutylammonium fluoride
THF	Tetrahydrofuran
TMEDA	Tetramethylethylenediamine
TGA	Thermal Gravimetric Analysis
TLC	Thin-Layer Chromatograph
TD-DFT	Time-dependent Density Functional Theory
TRPL	Time-resolved Photoluminescence
$SnCl_2$	Tin(II) chloride
NEt_3	Triethylamine
TFA	Trifluoroacetic acid
TIPS	Triisopropylsilyl
$AsPh_3$	Triphenylarsine
T_1	Triplet excited state
T_n	Triplet excited states
TZ	Triple Zeta
$Pd_2(dba)_3$	Tris(dibenzylideneacetone)dipalladium(0)
UV-Vis	UltraViolet-Visible
VR	Vibrational relaxation
$Zn(OAc)_2•2H_2O$	Zinc acetate dehydrate
ZnTPP	Zinc tetraphenylporphyrin

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